

**Hamiltonian dynamics of a quantum of space:
hidden symmetries and spectrum of the volume operator,
and discrete orthogonal polynomials**

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Abstract

The action of the quantum mechanical volume operator, introduced in connection with a symmetric representation of the three-body problem and recently recognized to play a fundamental role in discretized quantum gravity models, can be given as a second order difference equation which, by a complex phase change, we turn into a discrete Schrödinger-like equation. The introduction of discrete potential-like functions reveals the surprising crucial role here of hidden symmetries, first discovered by Regge for the quantum mechanical $6j$ symbols; insight is provided into the underlying geometric features. The spectrum and wavefunctions of the volume operator are discussed from the viewpoint of the Hamiltonian evolution of an elementary “quantum of space”, and a transparent asymptotic picture emerges of the semiclassical and classical regimes. The definition of coordinates adapted to Regge symmetry is exploited for the construction of a novel set of discrete orthogonal polynomials, characterizing the oscillatory components of torsion-like modes.

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I. INTRODUCTION

Extension of familiar angular momentum theory to describe quantum dynamics as a function of discrete variables is required to cope *e.g.* (i)-with structure and reactivity in molecular, atomic and nuclear physics [1, 2], (ii)-with use in quantum chemistry of elliptic coordinates and orbitals [3, 4], (iii)-with spin network approaches to quantum gravity [5, 6]. These approaches exploit progresses in understanding solvability of quantum systems, such as provided by dynamical symmetry algebras [2, 7].

An elementary spin network picture is schematized in Fig. 1: alternatively to the traditional sequential coupling of angular momenta, the volume operator $K = \mathbf{J}_1 \cdot \mathbf{J}_2 \times \mathbf{J}_3$, first defined in [8], acts democratically on vectors \mathbf{J}_1 , \mathbf{J}_2 and \mathbf{J}_3 plus a fourth one, \mathbf{J}_4 , which closes a (not necessarily planar) quadrilateral vector diagram $\mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 + \mathbf{J}_4 = 0$. Matrix elements of K were computed in [9] to provide a Hermitian representation, whose features have been studied by many [10–12] (see also [13] for an approach based on Bohr-Sommerfeld quantization). Carbone et al. [14] gave a geometrically based (Ponzano-Regge [15], Schulten-Gordon [16]) WKB asymptotics.

In this work, by a suitable complex change of phase, we transform the imaginary anti-symmetric representation into a real, time-independent Schrödinger equation which governs the Hamiltonian dynamics as a function of a discrete variable denoted ℓ . The Hilbert space spanned by the eigenfunctions of the volume operator [17] is constructed combinatorially and geometrically, applying polygonal relationships to the two quadrilateral vector diagrams in Fig. 1, which are “conjugated” by a hidden symmetry discovered by Regge [18]. We analyze the consequences of this elusive and other symmetries, providing a perspective geometrical view, helpful for both the characterization of molecular spectra and torsion-like modes, and also for the extraction of the polynomial components of rotovibrational wavefunctions.

II. DISCRETE SCHRÖDINGER EQUATION AND REGGE SYMMETRY

Eigenvalues k and eigenfunctions $\Psi_\ell^{(k)}$ of the volume operator are most simply obtained through the three-terms recursion relationship first introduced in [9] and analyzed in [14], where analytical expressions of eigenvalues k and eigenvectors $\Psi_\ell^{(k)}$ are given for Hilbert spaces up to dimension five. We follow the notation and units of reference [14], but find

it crucial to apply a change of phase $\Psi_\ell^{(k)} = (-i)^\ell \Phi_\ell^{(k)}$ to obtain a real, finite-difference Schrödinger-like equation

$$\alpha_{\ell+1} \Phi_{\ell+1}^{(k)} + \alpha_\ell \Phi_{\ell-1}^{(k)} = k \Phi_\ell^{(k)}. \quad (1)$$

The Φ_ℓ^k are the eigenfunctions of the volume operator expanded in the $\mathbf{J}_{12} = \mathbf{J}_1 + \mathbf{J}_2$ basis¹. The matrix elements α_ℓ in (1) are given in terms of geometric quantities, namely

$$\alpha_\ell = \frac{F(\ell; j_1 + 1/2; j_2 + 1/2) F(\ell; j_3 + 1/2; j_4 + 1/2)}{\sqrt{(2\ell + 1)(2\ell - 1)}}, \quad (2)$$

where $F(A, B, C) = \frac{1}{4}[(A + B + C)(-A + B + C)(A - B + C)(A + B - C)]^{\frac{1}{2}}$ is the Archimedes' ("Heron's") formula for the area of a triangle with side lengths A, B and C . Thus α_ℓ is proportional to the product of the areas of the two triangles sharing the side of length ℓ and forming a quadrilateral of sides $j_1 + \frac{1}{2}, j_2 + \frac{1}{2}, j_3 + \frac{1}{2}$ and $j_4 + \frac{1}{2}$, the parameters entering in Eq. (2)². Note that the latter physically correspond to four quantum numbers associated to the quantum angular momenta $\mathbf{J}_1, \mathbf{J}_2, \mathbf{J}_3$ and \mathbf{J}_4 . They appear to be all on the same footing, indicating that the volume operator can be thought of as acting democratically on either a composite system of four objects with vanishing total angular momentum, or a system of three objects with total angular momentum \mathbf{J}_4 .

The similarities between the discrete Schrödinger equation and the three-term recursion occurring for the $6j$ symbol motivated the authors of [14] to carry out the analysis of its semiclassical behavior along the lines of [15, 16]. Another similarity with the case of the $6j$ symbol appears concerning the range of ℓ . As noted in [17], the basic requirement that the four vectors form a (not necessarily planar) quadrilateral leads to identify the range of ℓ with

$$D = 2 \cdot \min(j_1, j_2, j_3, j_4, j'_1, j'_2, j'_3, j'_4) + 1 \quad (3)$$

which is also the dimension of the Hilbert space where the volume operator acts. Here j_i and j'_i are conjugated by Regge symmetry (Fig. 1), *i.e.* connected by $j'_i = s - j_i$, where

$$s = (j_1 + j_2 + j_3 + j_4) / 2 = (j'_1 + j'_2 + j'_3 + j'_4) / 2 \quad (4)$$

¹ The treatment would be analogous had we chosen the $\mathbf{J}_{23} = \mathbf{J}_2 + \mathbf{J}_3$ basis, with $\tilde{\ell} = j_{23}$. This construction relies on properties of the quadratic operator algebra generated by $(\mathbf{J}_{12})^2$, $(\mathbf{J}_{23})^2$ and K . Once chosen the eigenbasis of $(\mathbf{J}_{12})^2$, the other two operators are also tridiagonal and have the form of Eq. (1).

² In Loop Quantum Gravity j_i labels eigenvalues of the area operator $8\pi L_p \gamma \sqrt{j_i(j_i + 1)}$, where L_p is the Planck length and γ is the Immirzi parameter (see *e.g.* [5, 13]).

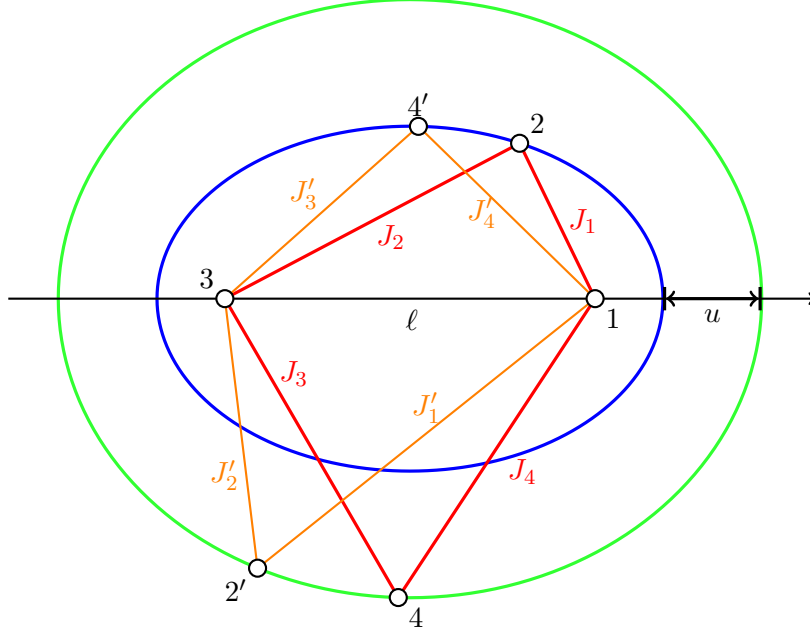


FIG. 1. A quadrilateral and its Regge “conjugate” illustrating the elementary spin network representation of the symmetric coupling scheme: each quadrilateral is dissected into two triangles sharing, as a common side, the diagonal ℓ . The other sides are of length $J_i = j_i + 1/2$ (and $J'_i = j'_i + 1/2$); ℓ , which is the discrete variable in Eq. (1), is shown as the distance between foci 1 and 3 of the confocal ellipses where the vertices of the quadrilaterals lie. The two sets of four side lengths of the Regge conjugate quadrilaterals are obtained by reflection with respect to the common semiperimeter s (Eq. (4)). This relationship can be interpreted either as concerted stretchings and shortenings by the parameter $r = (j_1 - j_2 + j_3 - j_4)/2$ introduced in [19], or by $v = (j_1 - j_2 - j_3 + j_4)/2$ occurring in the projective interpretation of Robinson [20]. Shown is also the difference between the semimajor axes of the two ellipses, $u = (j_1 + j_2 - j_3 - j_4)/2$. Signs are decided according to the choice of primed and unprimed quadrilaterals. Also, u and v would exchange their roles had we chosen the other diagonal $\tilde{\ell}$ as the variable ℓ (see note 1). In Eq. (11) the orthogonal nature of this set of transformations is exhibited explicitly by the matrix W . The passage to the Regge conjugate configuration $(s, -u, -r, -v)$ is revealed as a quaternionic conjugation, motivating our nomenclature.

is the semiperimeter, common to both quadrilaterals. The map between primed and un-

primed j s is given by the symmetric $O(4)$ transformation in

$$\frac{1}{2} \begin{pmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{pmatrix} \begin{pmatrix} j_1 \\ j_2 \\ j_3 \\ j_4 \end{pmatrix} = \begin{pmatrix} j'_1 \\ j'_2 \\ j'_3 \\ j'_4 \end{pmatrix}, \quad (5)$$

denoted R in the following. This is a striking manifestation of the relevance of the Regge symmetry in the present analysis: indeed it can be checked that the volume operator is invariant under such symmetry and therefore its spectrum and eigenfunctions are invariant too. The Regge symmetry shows up also to be important to assist in determining ranges of ℓ and of the j s. From Eq. (3) one can decide to work with unprimed quantities, label as j_1 the minimum of the eight entries and ordering j_2 and j_4 according to $j_1 \leq j_2 \leq j_4$; then $j_2 - j_1 = \ell_m \leq \ell \leq j_1 + j_2 + 1 = \ell_M$ and $j_4 - j_2 + j_1 \leq j_3 \leq j_4 + j_2 - j_1$. The lower and upper limits in j_3 correspond respectively to $u = 0$ and $r = 0$, *i.e.* cases when the two Regge conjugate quadrilaterals are coincident.

III. HAMILTONIAN DYNAMICS

Transparent techniques are available to study the semiclassical behavior of difference equations of type (1) (see. *e.g.* [21, 22] and references therein). The Hamiltonian operator for the discrete Schrödinger equation (1) can be written, in terms of the shift operator $e^{\pm i\varphi} \Phi_{\ell}^{(k)} = \Phi_{\ell \pm 1}^{(k)}$,

$$\hat{H} = (\alpha_{\ell} e^{-i\varphi} + \alpha_{\ell+1} e^{i\varphi}) \quad \text{with} \quad \varphi = -i \frac{\partial}{\partial \ell} \quad (6)$$

representing the variable canonically conjugate to ℓ . The two-dimensional phase space (ℓ, φ) supports the corresponding classical Hamiltonian function given by

$$H = 2\alpha_{\ell+\frac{1}{2}} \cos \varphi, \quad (7)$$

as illustrated in Fig. 2 for the two Regge conjugate quadrilaterals of Fig. 1, now allowed to fold along ℓ with φ perceived as a torsion angle³.

³ Similarly the dependence on ℓ can be appreciated as a concerted bending mode, for example writing the product of the areas in the numerator of Eq. (1) as $(J_1 J_2 J_3 J_4 \sin \theta_1 \sin \theta_3)/4$, where θ_1 and θ_3 are internal angles in 1 and 3, respectively.

The classical regime occurs when quantum numbers j s are large and ℓ can be considered as a continuous variable. This limit for α_ℓ permits us to draw the closed curves in the (ℓ, k) plane of Fig. 3 and Fig. 4, obtained when $\varphi = 0$ or π in Eq. (7). These curves have the physical meaning of torsional-like potential functions

$$U_\ell^+ = -U_\ell^- = 2\alpha_\ell, \quad (8)$$

viewing the quadrilaterals in Figs. 1 and 2 as mechanical systems. Noteworthy in Fig. 3 is the further symmetry along the $k = 0$ line ($\varphi = \pi/2$), missing *e.g.* in the otherwise similar case of $6j$ symbol [19], where “caustic curves” are studied in a square of the (j_{12}, j_{23}) plane (the “screen”). Here the perfect duality between j_{12} and j_{23} is lost, and the symmetry along the $k = 0$ line appears in the potential functions as the continuous counterpart of the known fact that eigenvalues of the volume operator come in pairs, k and $-k$ (plus possibly the $k = 0$ eigenvalue when D is odd). Another manifestation of this symmetry links the eigenfunctions: it is easy to show from Eq. (1) that $\Phi_\ell^{(k)} = (-1)^\ell \Phi_\ell^{(-k)}$, and this appears in Fig. 3 as the striking alternating features in the positive part of the spectrum⁴.

The phenomenology of caustics presented in [19] can be interestingly translated to this case, but taking into account also such additional symmetries. Remarkably Regge symmetry is a key to the classification of the Lissajous-type of potential functions given in Eq. (8). This includes also the limits where some quantities are large, which in the $6j$ case lead to the $3j$ ’s [19]. In the present case this limiting procedure can be shown to lead to the cylindrical or planar spin networks discussed by Neville [23] for unpolarized and polarized gravitational waves.

IV. DISCRETE ORTHOGONAL POLYNOMIALS

The preceding considerations apply to the interesting issue of extracting the polynomial components out of wavefunctions and to this aim the defining three-term recursion in Eq. (1) is sufficient according to Favard theorem [24]. Actually, these polynomials can be obtained from the secular equation once eigenvalues are calculated. However, instead that directly from Eq. (1), we find it much more insightful (*i*) - to eliminate the square roots to give an

⁴ The “mirror” symmetry of the $6j$ enlightened in [19] applies here too. In particular, allowing negative values of ℓ would permit infinite replicas of Figs. 3 and 4 on both sides of the ℓ range.

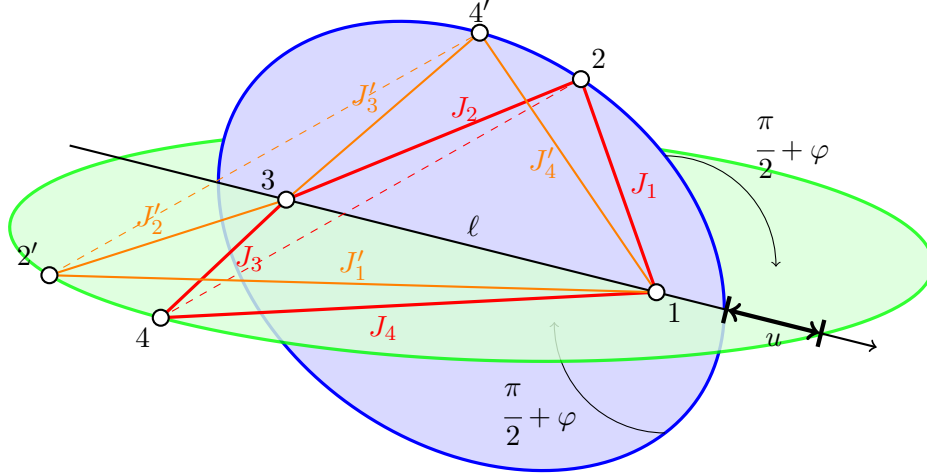


FIG. 2. The two quadrilaterals of Fig. 1, looked at as a mechanical system, evolve creasing the pairs of triangles in which are dissected along ℓ , according to a torsion mode corresponding to the same dihedral angle $\frac{\pi}{2} + \varphi$ in both cases. Adding the edges $\overline{24}$ and $\overline{2'4'}$ two tetrahedra having the same volume can be visualized. In fact, their volume is proportional to H of Eq. (7) which is the product of the areas of two triangles divided by the length of the hinging edge times the sine of the dihedral angle. Thus classically the volume is an energy function which is a constant of motion along the classical trajectories which are solutions of the Hamilton equations $\frac{d\ell}{dt} = \frac{\partial H}{\partial \varphi}$; $\frac{d\varphi}{dt} = -\frac{\partial H}{\partial \ell}$. Indeed, edges $\overline{24}$ and $\overline{2'4'}$ would have the same length $\tilde{\ell} = j_{23}$ had we chosen to expand the volume operator in the basis of $\mathbf{J}_{23} = \mathbf{J}_2 + \mathbf{J}_3$ (note 1): two different confocal ellipses would describe the system and the vertices 2, 4 would coincide with 2', 4' as the foci of the new ellipses. On the other hand, vertices 1 and 3 would split to give 1' and 3', say, lying on the new ellipses and belonging either to a quadrilateral or to its conjugate.

unsymmetrical three-term recursion with polynomial coefficients; this leads at each step to a polynomial proportional to $\Phi_\ell^{(k)}$ within a normalizing factor and a phase convention; (ii) - to impose Regge invariance as a guideline to obtain an illuminating geometrical interpretation, specifically that of two triangles forming a tetrahedron, the two faces being hinged in a common side, and having respectively s and u , or r and v , as the other sides; (iii) - to show that the requirement of polynomial coefficients highlights the role of the new variables s, u, r, v , introduced on a purely geometrical ground in Fig. 1. After some algebra, we obtain from Eq. (1) the following unsymmetrical three-term relation, which is manifestly Regge

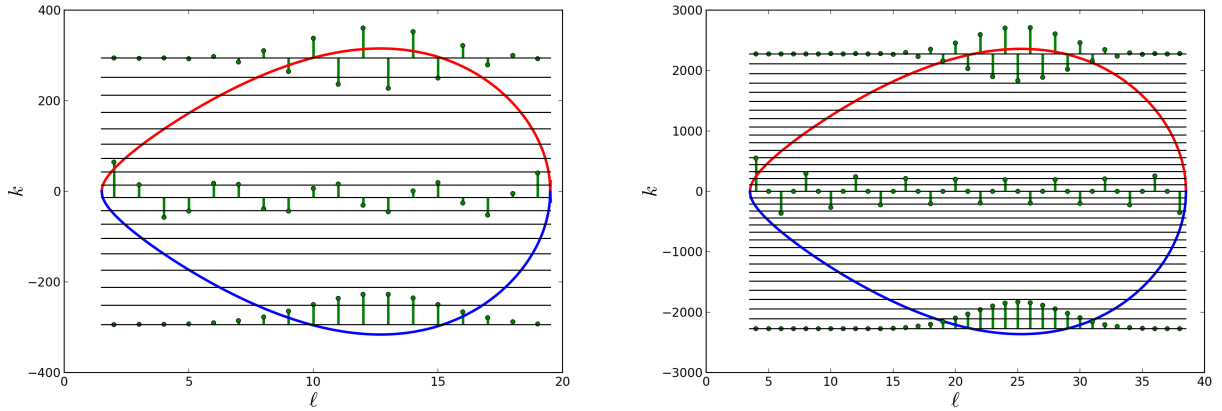


FIG. 3. Two examples of spectra of the volume operator: the horizontal lines represent the eigenvalue k , the curves are the caustics (the turning points of the semiclassical analysis), which limit the classically allowed region (in red U_ℓ^+ , in blue U_ℓ^- Eq. (8)). As can be seen, the eigenvalues are symmetrically distributed with respect to the $k = 0$ (which is an eigenvalue if D is odd). In green the stick graph of three of the eigenfunctions (unnormalized). Left: parameters $j_1, j_2, j_3, j_4=8.5, 10.5, 13.5, 14.5$ or $s, u, r, v=23.5, -4.5, 1.5, 0.5$. Right: all four parameters are doubled. The extrema of U_ℓ^+ and U_ℓ^- bracket the spectrum, which can be well understood analytically and confirmed by extensive numerical checks. The characteristic features of U_ℓ^+ and U_ℓ^- can be compared to those for the caustics for the $6j$ symbol [19].

invariant and has polynomial coefficients

$$(2\ell + 1) F^2(s, u, \ell - 1) p_{\ell-1}^{(k)} + (2\ell - 1) F^2(r, v, \ell + 1) p_{\ell+1}^{(k)} = k (4\ell^2 - 1) p_\ell^{(k)}. \quad (9)$$

The relation between $p_\ell^{(k)}$ and the $\Phi_\ell^{(k)}$ of Eq. (1) is given by

$$p_\ell^{(k)} = N_\ell \Phi_\ell^{(k)} \text{ and } N_{\ell-1} = \frac{F(s, u, \ell - 1)}{F(r, v, \ell)} N_\ell, \quad (10)$$

a two-term relation which can be solved in closed form, see *e.g.* [4]. Normalization can be chosen by setting boundary conditions (*e.g.* $p_{\ell_m}^{(k)} = 1$, $p_{\ell_m-1}^{(k)} = 0$).

V. CONCLUDING REMARKS AND OUTLOOK

In retrospect, we have introduced a linear transformation R which maps the two Regge conjugated quadrilaterals, Eq. (5), and another transformation W which defines the new

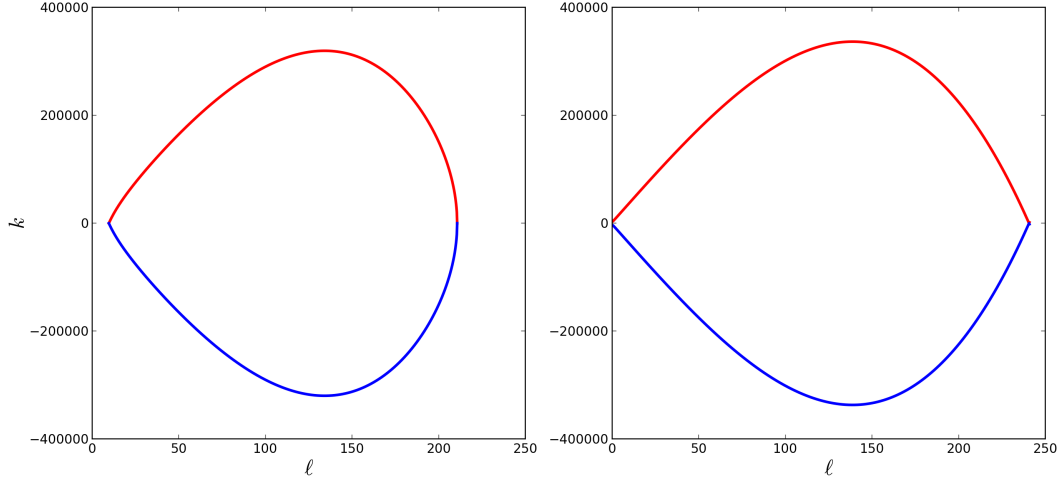


FIG. 4. Potential functions U^+ and U^- (Eq. (8)) are shown for two cases where the conjugated tetrahedra coincide. The cases occur when (i) - $r = 0$ (i.e. $j_1 + j_3 = j_2 + j_4$) (ii) - $u = 0$ ($j_1 + j_2 = j_3 + j_4$). (iii) $v = 0$ ($j_1 + j_4 = j_2 + j_3$). From the viewpoint of Fig. 2, case (i) would correspond to a “tangential” quadrilateral, while (ii) and (iii) to “ex-tangential” ones. In the left panel, case where only one of the r, u, v variables is zero ($j_1, j_2, j_3, j_4 = 100.0, 110.0, 130.0, 140.0$, $v = 0$), while on the right all three of them are zero. The latter is the case for an equilateral quadrilateral $j_1 = j_2 = j_3 = j_4 = 120.0$ (compare to [19] for the analogous cases which appear in the discussion of the 6j symbol).

variables (Fig. 1)

$$\frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix} \begin{pmatrix} j_1 \\ j_2 \\ j_3 \\ j_4 \end{pmatrix} = \begin{pmatrix} s \\ u \\ v \\ r \end{pmatrix}. \quad (11)$$

The matrix W is recognized as the famous one which provides atomic “hybrids” of tetrahedral symmetry by combining one s and three p hydrogenoid orbitals [25]. Also, the (s, u, r, v) parametrization is reminiscent of kinematic rotations [26] of the quadrilaterals whose edges are interpreted as distances among four equal mass bodies.

Summarizing, the hidden Regge symmetry acts on the new variables in an interesting

way

$$\begin{array}{ccc}
 (j_1, j_2, j_3, j_4) & \xrightleftharpoons{R} & (j'_1, j'_2, j'_3, j'_4) \\
 \updownarrow W & & \updownarrow W \\
 (s, u, r, v) & \xrightleftharpoons{Q} & (s, u', r'v')
 \end{array} \tag{12}$$

where $WRW = Q = \text{diag}(1, -1, -1, -1)$. Therefore the transformation W and the introduction of new variables permit to associate a quaternion and its conjugate to the two quadrilaterals twinned by Regge symmetry. Implications of this remark in the mathematical context of dynamical algebras will be addressed elsewhere.

Regarding the quadrilaterals in Figs. 1 and 2 as mechanical devices, note that the u , v and r coordinates are interestingly analogous to parameters occurring in the Grashof classification of four-bar linkages [27], the elementary moving mechanism of engines. For example, the conditions for identify of Regge conjugates, namely that at least one of them be zero, are those for the full folding of the mechanism.

The educated guess that equivolume Regge conjugated tetrahedra are scissor congruent eluded a constructive proof so far [28]: our construction (Fig. 2) works by creasing along a diagonal the two plane isoperimetric quadrilaterals of Fig. 1, concertedly stretched by either r or u or v . The quadrilaterals are not scissor congruent: each is dissected into two triangles, with congruency with respect to the product, not the sum, of their areas.

The discrete orthogonal family of polynomials of section IV is not “classical”, *i.e.* does not belong to the hypergeometric families of the Askey schemes (see [29] for relevance in applied quantum mechanics). Suitable generalizations would be interesting to be developed: indeed, the situation is similar to that encountered for the Mathieu, Ince, Lamé and Heun families occurring for the separation of variables in elliptic coordinates for the action of the Laplacian operator on compact manifolds, see e.g. [4, 30]. Limiting cases can be formulated accordingly, such as the cylindrical or planar spin networks [23], or the q extensions⁵.

This set of issues, besides the cases outlined here, appears to be relevant to special function theory, with particular reference to the development of orthogonal basis sets of interest in applied quantum mechanics, and specifically in atomic and molecular physics, and in quantum chemistry.

⁵ The q extensions can be conveniently based on the formulation of α_ℓ in Eq. (2) as a product of two $6j$'s [9] for which the q -extension is well established

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